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Rotational analysis of the β-system of BO

By Albin Lagerqvist, N. E. Lennart Nilsson and Kurt Wigartz

With 2 figures in the text

ABSTRACT

Rotational analyses of nine bands of the $\beta(B\,{}^2\Sigma^+\text{–}X\,{}^2\Sigma^+)$ system of BO have been carried out. Rotational and vibrational constants have been derived. The constants for the upper level, $B\,{}^2\Sigma^+$, are as follows:

$$B'_v = 1.5171 - 0.0210\,(v' + \tfrac{1}{2})\ \text{cm}^{-1}; \quad r'_e = 1.3053 \times 10^{-8}\ \text{cm}$$
$$D'_e = 8.5 \times 10^{-6}\ \text{cm}^{-1}$$
$$\omega'_e = 1281.69 \quad ; \quad \omega'_e x'_e = 10.66$$
$$T'_e = 43174.05.$$

A survey of the spectroscopic data for BO is given.

Introduction

BO has two well-known bandsystems, the α-system representing a ${}^2\Pi\text{–}{}^2\Sigma^+$ transition and lying in the visible region and the β-system, which is a ${}^2\Sigma^+\text{–}{}^2\Sigma^+$ transition and situated in the ultraviolet. The lower ${}^2\Sigma^+$ state is the same for the two transitions and is probably the ground state. Fine structure analyses of the α-bands have been carried out by Jenkins (1927), Scheib (1930) and Jenkins and McKellar (1932). The latter authors studied in particular the mass ratio of the boron isotopes. As source they used BCl_3 vapor mixed with a stream of active nitrogen containing traces of oxygen. Scheib developed the α-bands in the arc, which owing to its higher temperature gives many more rotational lines.

Mulliken (1935) investigated the vibrational isotope effect of the α and β bands excited in active nitrogen.

The first rotational analysis of the β-system was performed by Elliot (1930). He analysed the 0,1 and 0,2 bands. He estimated B'_0 to be about 1.53 cm^{-1}. This value is too high and seems to be a misprint. Thus, Herzberg (1950) gives the value 1.503 with reference to this paper by Elliot (1930). Elliot examined the β-bands in the arc. He used a quartz spectrograph, in which the inverse dispersion in the actual region (2400–2600 Å) was about 3 Å/mm. Elliot found two R and two P branches.

In 1935 Funke and Simons made a rotational analysis of four β-bands, namely the 1,0, 0,0, 0,1 and 0,2 bands. They reported that they were not able to resolve the spin doubling, though they used a grating spectrograph having a dispersion which was 30 % greater than that of Elliot's quartz spectrograph. They found $B'_0 = 1.51$ and $B'_1 = 1.49$. Their observed B'' values agree very poorly with those given by Jenkins.

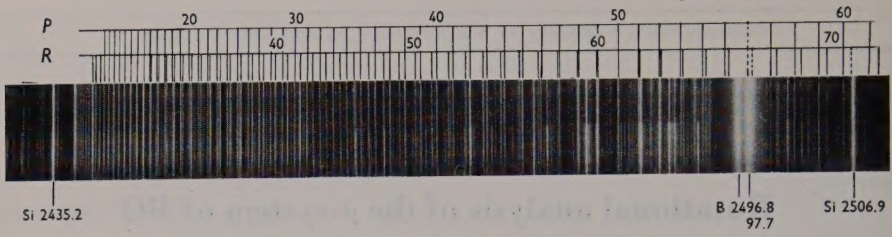

Fig. 1. Reproduction of the 0,1 band of the β-system.

They considered that the poor agreement arose from uncertainties in the Fe standards in the ultraviolet region (the 1,0 band lies at λ 2265 Å) and from the blending of many lines near the *R* heads.

Elliot (1935) published a note on the β-bands, where he gave the wavenumbers for some lines of the 0,1 and 0,2 bands, showing the doubling effect. Neglecting the spin doubling in the ground state he determined the spin constant γ' to be about 0.02 cm^{-1}.

Thus our knowledge of the β bands is not great. For this reason we have performed a more thorough analysis of the β-system.

The BO spectrum is of astrophysical interest as there is evidence that the α-bands are present in the solar spectrum (Broida and Moore (1957)).

Experimental

The source of light was a carbon arc, whose lower positive electrode contained amorphous boron. It was run at a current of about 4 A from a 220 V.D.C. supply. The spectrograms were taken in a first order of a Wood's 21 ft concave grating (165000 lines in all). The inverse dispersion is about 1.3 Å/mm in the actual region (2200–2600 Å). Kodak 103-O plates were used. Several exposures with different exposure times (1 to 4 hours) were made. Iron lines, whose wavelengths were taken from the M.I.T. Tables (1939) and Lofthus' Tables (1956) were used for comparison.

Structure of the bands

The bands show the appearance typical of a $^2\Sigma$–$^2\Sigma$ transition. Thus two *R* and two *P* branches are present. At small *K*-numbers the doublets are not be resolved. Fig. 1 gives a reproduction of the 0,1 band. No effort has been made to measure the $B^{10}O^{16}$ lines, only lines belonging to the most abundant istopes $B^{11}O^{16}$ have been measured. The following bands have been analysed: 3,1, 2,0, 2,2, 1,0, 1,4, 0,0, 0,1, 0,2 and 0,3. The wavenumbers of the lines are given in tables 1–5. Overlapped lines are indicated with an asterisk. The accuracy is about 0.05 cm^{-1} for most lines, but considerably worse for overlapped and weak lines. The accuracy increases to longer wavelengths. Only a few lines of the 3,0 band could be detected.

Attempts have been made to decide which *R* and *P* branches arise respectively from F_1 and F_2 levels. From intensity relations we know that an F_1 line is a little more intense than the F_2 line. This difference increases with decreasing *K* number. Microphotometer traces of some bands did not give a definite answer. The assignment chosen in table 1–5 is that used earlier. The traces, however, give some slight indication that this arrangement may be the wrong one.

Table 1. Wavenumbers for the lines of the 0,1 and 0,2 bands.

K	0,1				0,2			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
5							39 149.73*	
6							43.90*	
7					39 182.84*		37.62*	
8					81.93*		30.77*	
9					80.93*		23.57*	
10					79.35*	79.04*	16.06	15.89
11	41 013.44*	012.93*			77.11	76.92	07.84	07.66
12	10.36*	10.00*	40 935.11	934.73	74.56	74.22	099.20	098.97
13	06.86*	06.40*	25.77	25.40	71.33	71.07	90.10	89.95
14	02.82*	02.47*	15.67	15.12	67.76	67.48	80.55	80.30
15	40 998.33*	997.86*	04.86	04.58	63.83	63.50	70.76	70.17
16	93.34*	92.86*	894.23	893.63	59.34	58.88	59.99	59.76
17	87.65*	87.26*	82.54	82.11	54.28	53.82	49.03	48.80
18	81.60*	81.18*	70.49	70.10	48.77	48.41	37.58	37.31
19	75.16*	74.59*	57.96	57.50	42.78	42.42	25.79	25.50
20	67.92*	67.35*	44.94	44.37	36.34	35.96	13.30	12.92
21	60.56*	59.94*	31.35	30.85*	29.38	28.87	00.38	999.97
22	52.31*	51.84*	17.38*	16.85*	22.06	21.51	39 987.04	86.66
23	43.31*	42.73*	02.91	02.25	14.25	13.59	73.29	72.88
24	34.28	33.69	787.61	787.09	05.77	05.10	58.95	58.57
25	24.60	23.88	72.13	71.48	39 096.89	096.20	44.34	43.69
26	14.56	13.88	55.80*	55.27*	87.53	86.85	29.05	28.53
27	03.74	03.19	39.35	38.70	77.66	76.96	13.29	12.84
28	892.44	891.75	22.33	21.65	67.34	66.72	897.09	896.42
29	80.53	79.88	04.69	03.89	56.52	55.73	80.42	79.74
30	68.28	67.58	686.35	685.84	45.16	44.35	63.19	62.53
31	55.49	54.68	67.73	67.05	33.27	32.49	45.56	44.88
32	41.84	41.09	48.42	47.63	20.99	20.16	27.38	26.76
33	28.03	27.11	28.63	27.91	08.11	07.43	08.75	08.02
34	13.58	12.70	08.23	07.74	38 994.72	993.96	789.61	788.90
35	798.52	797.67	587.61	586.84	80.87	80.11	70.00	69.33
36	83.03	82.15	66.20	65.56	66.57	65.71	49.95	49.20
37	66.90	66.10	44.60	43.61	51.68	50.79	29.34	28.56
38	50.18	49.32	22.11	21.30	36.31	35.51	08.27	07.46
39	33.20*	32.33	499.24	498.29	20.44	19.46	686.61	685.79
40	15.33	14.39	75.94	74.87	03.93	03.11	64.64	63.71
41	697.12	696.11	51.87	50.93	887.11	886.22	41.73	41.09
42	78.24	77.31	27.35	26.35*	69.66	68.76	18.80	17.81*
43	58.90	57.99	02.32	01.37	51.76	50.72	595.21	594.20*
44	38.88	37.93	376.63	375.70	33.17	32.26	71.07	70.20
45	18.40	17.29	50.69	49.57	14.23	13.19	46.48	45.54
46	597.37	596.22	23.91	22.93	794.75	793.62	21.31	20.28
47	75.73	74.58	296.81	295.71	74.58	73.65	495.69	494.89
48	53.40	52.51	69.04	67.94	53.97	52.95	69.55	68.50
49	30.76	29.66	40.56*	39.56	32.90	31.85	42.88	41.86
50	07.37	06.21	11.83*	10.63*	11.16	10.12	15.61	14.63
51	483.41	482.32	182.30	181.24*	688.84	687.82	387.79	386.86
52	58.89	57.84	52.50	51.25	66.10	65.04	59.58	58.52
53	33.92	32.76	21.82	20.76	42.80	41.91	30.81	29.77
54	08.13	06.92	090.77	089.53	19.01	17.81*	01.55	00.49

Table I. (*continued*)

K	0,1				0,2			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
55	40 381.94	380.71	—	—	38 594.44*	593.32	38 271.67	270.60
56	55.11	53.82	—	—	69.35	68.39	—	40.16
57	27.53	26.41	39 993.89	992.80	—	—	10.29	09.21
58	299.59	298.27	60.55	59.36	17.85	16.74	178.89	177.80
59	71.01	69.69	26.47	25.35	491.07	489.90	46.87	45.71
60	41.48	40.56*	891.99	890.67	63.86	62.58	14.28	13.08
61	11.83*	10.63*	56.83	55.62	36.00	34.81	081.20	079.95
62	181.24*	179.96	21.10	19.83	07.62	06.34	47.53	46.28
63	50.21	48.96	784.73	783.64	378.61	377.31	13.29	11.98
64	18.45	17.10	47.94	46.68	49.17	47.67	37 978.47	977.23
65	086.35*	084.88	10.35	09.12	18.84	17.55	43.07	41.79
66	—	—	672.34	671.14	288.03	286.81	07.28*	05.91
67	—	—	33.37	32.33	56.76	55.46	870.90*	869.50*
68	39 985.26	983.92	594.18	592.99	24.81	23.35	33.52	32.24*
69	50.45*	49.14*	54.55	53.11	192.12	190.69*	796.09	794.86
70	14.83	13.54	13.91	12.51	58.97	57.61	57.82	56.50
71	—	—	472.67	471.37	25.15	23.77	19.03	17.69
72	842.01	840.54	31.04	29.65	090.76	089.39	679.57*	678.29*
73	04.40	03.06	388.61	387.29	55.73	54.32	39.64	38.28
74	766.34	764.77	45.50	44.20	19.87	18.54	599.02	597.72
75	27.45	26.07	01.84	00.48	37 983.61	982.32	57.94	56.45
76	688.11	686.71	257.56	256.21	46.77	45.41	16.13	14.72
77	47.99	46.54	12.31	11.30	09.24*	07.83*	473.80	472.35
78	07.19	05.72	167.13	165.66	870.90*	869.50*	30.69	29.32
79	565.68	564.38	20.88	19.47	32.24*	30.74	387.15	385.74
80	23.71	22.27	073.92	072.44	792.59*	791.19	43.06	41.70
81	480.73	479.26	26.56	24.96	52.58	50.91	298.11	296.65
82	37.29	35.88			11.52*	10.14	52.65	51.21
83	393.08	391.53			670.26	668.73	06.54	05.16
84	48.07	46.53						
85	02.55	00.93						
86	256.15	254.48						
87	08.91	07.51						

Evaluation of rotational and vibrational constants

Approximate B and D values have been determined by means of the usual graphical method by plotting $\frac{\Delta_2 F(K)}{4(K+\frac{1}{2})}$ against $(K+\frac{1}{2})^2$. Here $\Delta_2 F(K)$ is the mean of $\Delta_2 F_1(K)$ and $\Delta_2 F_2(K)$. The best experimental data have been obtained for the level $v'=0$, which is the upper state for four of the investigated bands. Choosing an approximate D_0' value and forming the expression

$$\frac{\Delta_2 F'(K)}{4(K+\frac{1}{2})} + 2D_0'(K+\tfrac{1}{2})^2$$

where the combination differences are the means obtained from the four bands, a good B_0' value has been calculated with the aid of least squares.

Table 2. Wavenumbers for the lines of the 0,0 and 1,0 bands.

K	0,0				1,0			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
7			42 836.44	836.09			44 096.17	
8	42 880.12*	879.91*	29.08	28.80			88.36	
9	78.36*	77.96*	21.29	20.95	44 136.86	136.37	80.44	
10	76.15*	75.76*	13.04	12.69	33.94	33.57	71.41	
11	73.26	73.00	04.05	03.72	30.43	29.85	62.20	61.82
12	69.74	69.45	794.65	794.20	26.51	26.16	52.40	51.80
13	65.81*	65.36*	84.76	84.48	22.17	21.41	41.99	41.35
14	61.35	60.97	74.27	73.92	16.87	16.40	30.90	30.22
15	56.23	55.85	63.23	62.80	11.25	10.76	19.37	18.81
16	50.67	50.31	51.73	51.33	04.91	04.32	07.08	06.38
17	44.56	44.13	39.61	39.19	097.83	97.28	43 994.36	993.74
18	37.92	37.51	26.83	26.50	90.48	89.80	80.91	80.22
19	30.56	30.08	13.59	13.35	82.27	81.67	67.06	66.32
20	22.92	22.45	00.14*	699.67	73.72	72.94	52.53*	51.93
21	14.56	14.06	685.84*	85.27	64.32	63.58	37.13*	36.03*
22	05.68*	05.07*	71.09*	70.52	54.52	53.86	21.47	20.91
23	796.26*	795.79*	55.36*	54.96*	44.11	43.41	05.49	04.74
24	86.37	85.73*	39.69*	39.00*	32.94	32.14	888.72*	887.89
25	75.75	75.16	23.30	22.81*	21.50	20.65	71.00*	70.31
26	64.77	64.15	06.50	05.80*	09.31	08.40	53.05*	52.34
27	53.17	52.60	588.75	588.09*	43 996.43	95.46	34.42*	33.75*
28	40.89	40.20	70.73	70.00	82.94	82.00	15.55	14.61*
29	28.10	27.68	52.03	51.44	69.05	68.10	795.21*	794.56*
30	15.02	14.22	33.01	32.27	54.23	53.18*	74.96	74.13*
31	01.01	00.30*	13.25	12.82	38.99	38.31*	53.93	52.82*
32	686.55	685.84*	493.03	492.27	23.03	22.11	32.50	31.74
33	71.60	71.09*	71.90	71.37	06.82	06.11	10.24	09.55
34	56.07	55.36*	50.72	49.91	889.58	88.72*	687.47	686.70
35	40.07	39.00*	28.76	27.99	71.87*	71.00*	63.98	63.28
36	22.81*	22.24	06.25	05.49	53.82	53.05*	40.25	39.19
37	05.59	04.82	383.25	382.42	34.42*	33.75*	15.67	14.76
38	587.81	586.85*	59.55	58.80	15.13	14.32*	590.15	589.24
39	69.30	68.39	35.40	34.54	794.56*	93.77*	64.40	63.60
40	50.45	49.27	10.73	09.95	73.96*	73.27*	38.39	37.35
41	30.71	29.63	285.25	284.24	52.82*	51.78	11.03	10.23
42	10.42	09.42	59.52	58.37	30.53	29.81	483.44	482.55
43	489.50	488.61	33.08*	32.02	08.13	07.29	54.97	54.14
44	68.24	67.27	06.06	04.93	684.68	83.76	26.30	25.43
45	46.24	45.14	178.41	177.49	60.87	59.69	396.95	395.95
46	23.65	22.50	50.14	49.06	36.22	35.15	66.59	65.82
47	00.43	399.34	21.44*	20.32	10.97	09.98	35.97	35.01
48	376.54	75.45	092.07	091.02	585.15	84.07	04.92	03.78
49	52.18	51.12	62.08*	60.99	58.67	57.70	272.78	271.67
50	27.18	26.14	31.62	30.54*	31.64	30.52	40.00	38.97
51	01.58	00.43	00.32	999.30	03.72	02.56	06.91	05.98
52	275.36	274.26*	—	—	475.16	474.12	173.14	172.06
53	48.51	47.36	41 936.46	35.28	46.18	45.08	38.53	37.51
54	20.89	19.76	03.66	02.46	16.38	15.20	03.40	02.44
55	192.89	191.61*	869.95	868.82	385.93	384.79	067.66	066.55
56	64.16	62.95	35.84	34.74	54.91	53.59	31.18	30.07

Table 2. (*continued*)

K	0,0				1,0			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
57	42 134.85	33.70	41 801.26	0.02*	43 323.03	22.07	42 994.12	993.32
58	04.99	03.73	765.94	764.86	290.64	289.34	56.73	55.21
59	074.42	073.09	29.90*	28.96*	58.60	56.29	18.28	17.04
60	43.33	41.94	693.57*	692.21*	23.80	22.51		
61	11.53	10.14			189.18	188.18		
62					54.40*	52.70		
63					18.35	17.18		
64					081.85	080.63		
65					44.46	43.31		
66					06.51	05.38		
67					42 967.97	966.92		
68					28.71	27.38		
69					888.82	87.39		

The origins ν_0 have been determined by use of the expression

$$2\nu_0 = R(K-1) + P(K) - 2(B' - B'')K^2 + 2(D' - D'')K^2(K^2+1). \qquad (1)$$

Approximate B', B'', D' and D'' values obtained from the graphical method have been put into this expression, which was plotted against K^2. Perfect rotational constants ought to give a horizontal line. ν_0 is obtained at $K^2 = 0$. The linear deviation gives $\Delta(B' - B'')$. At higher K^2 values a square deviation can be observable giving $\Delta(D' - D'')$.

The α values have been checked by calculating the vibrational differences $G(v+1) - G(v)$. The following expression was used for lines having the same upper state

$$\tfrac{1}{2}[R_{v'v''_1}(K) - R_{v'v''_2}(K) + P_{v'v''_1}(K) - P_{v'v''_2}(K)] =$$

$$= G''(v''_2) - G''(v''_1) - (B_{v''_1} - B_{v''_2})K(K+1) + (D_{v''_1} - D_{v''_2})K^2(K+1)^2 \qquad (2)$$

and the following for lines having the same lower state

$$\tfrac{1}{2}[R_{v'_2v''}(K-1) - R_{v'_1v''}(K-1) + P_{v'_2v''}(K+1) - P_{v'_1v''}(K+1)] =$$

$$= G'(v'_2) - G'(v'_1) - (B_{v'_1} - B_{v'_2})K(K+1) + (D_{v'_1} - D_{v'_2})K^2(K+1)^2 \qquad (3)$$

In the first expression

$$B_{v''_1} - B_{v''_2} = (v''_2 - v''_1)\,\alpha''$$

$$D_{v''_1} - D_{v''_2} = (v''_2 - v''_1)\,\beta''$$

In the second expression

$$B_{v'_1} - B_{v'_2} = (v'_2 - v'_1)\,\alpha'$$

$$D_{v'_1} - D_{v'_2} = (v'_2 - v'_1)\,\beta'$$

Table 3. Wavenumbers for the lines of the 0,3 and 1,4 bands.

K	0,3				1,4			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
4			37 340.63	340.41				
5			35.40	34.95			36 805.06*	
6			30.03	29.68			799.54	799.20
7			23.84	23.59			93.31	92.96
8	37 368.35*		17.30	17.02			86.69*	
9	67.66	67.45	10.39	10.10			79.93	79.63
10	66.42	66.06	03.04	2.73			72.41	72.10
11	64.67	64.23	295.39	295.04			64.48	64.22
12	62.49	62.03	87.12	86.78	36 830.35*		56.35	56.05
13	59.74	59.32	78.54	78.10	27.54*		47.57	47.23
14	56.60	56.14	69.47	69.08	24.24*		38.28	37.90
15	52.99	52.58	59.90	59.50	20.44*		28.61	28.14
16	48.98	48.61	49.76	49.47	16.25*		18.54	18.19
17	44.59	43.98	39.44	39.08	11.83*		08.17*	07.66*
18	39.71	39.21	28.52	28.10	06.65	06.32	697.31*	696.85
19	34.28	33.85	17.34	16.98	01.06	00.60	85.94*	85.44
20	28.57	28.01*	05.62	05.14	795.10	794.65	73.93*	73.47
21	22.40	21.83	193.43	192.99	88.62	88.16	61.49*	61.02
22	15.70	14.97	80.85	80.35	81.66	81.18	—	—
23	08.59	07.80	67.81	67.22	74.24	73.66	35.13	34.66
24	00.89	00.26	54.30	53.82	—	65.86	21.66*	21.19
25	292.91	292.27	40.26	39.73	58.12	57.55	07.66*	07.02
26	84.38	83.69	25.90	25.39	49.38	48.72	593.16	592.50
27	75.47	74.66	11.00	10.49	40.13	39.42	78.01	77.41
28	66.12	65.33	095.69	095.09	30.36	29.67	62.42	61.87
29	56.14	55.40	80.00	79.37	20.17	19.48	46.58	45.82
30	45.78	45.09	63.92	63.23	09.49*	08.85*	30.25	29.48
31	35.03	34.22	47.30	46.61	698.36	697.67	13.41	12.63
32	23.80	22.97	30.21	29.47	86.84	85.98*	496.05	495.27
33	12.03	11.15	12.67	11.97	74.75	73.95*	78.35	77.46
34	199.76	198.98	36 994.68	993.93	62.19	61.47*	59.91	59.12
35	87.11	86.22	76.21	75.40	49.07	48.32	41.23	40.46
36	73.95	73.12	57.26	56.50	35.63	34.95	22.02	21.23
37	60.34	59.52	37.84	37.13	21.62*	20.88	02.30	01.50
38	46.23	45.34	18.06*	17.28	07.23*	06.27	382.15	381.31
39	31.63	30.72	897.79	897.02*	592.17	591.32	61.52	60.61
40	16.59	15.65	76.98	76.12	76.68	75.81	40.44	39.61
41	0.99	00.08	55.73	54.85	60.72	59.84	18.88	18.02*
42	084.94	083.97	33.96	33.13	44.31	43.40	296.88	295.92*
43	68.41	67.37	11.66	10.93	27.36	26.40	74.34	73.41
44	51.40	50.40	789.13	788.27	09.89	08.88	51.27	50.40*
45	33.89	32.86	65.92	65.07	491.87	490.86	27.79	26.82
46	15.89	14.89	42.41	41.60	73.39	72.42	03.93	02.91
47	36 997.39	996.28	18.34	17.39	54.45	53.45	179.41	178.44
48	78.36	77.29	693.81	692.80	35.00	33.95	54.38	53.37
49	58.81	57.69	68.74	67.65	15.01	13.98	28.93	27.96
50	38.71	37.66	43.25	42.21	394.44	393.35	2.92	01.91
51	18.06*	17.05	17.19	16.17	73.42	72.34	076.53	75.50
52	897.02*	896.03	590.69	589.60	51.76	50.64	49.61	48.65*
53	75.59	74.49	63.69	62.68	29.69*	28.67	22.17*	21.08

Table 3. (*continued*)

K	0,3				1,4			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
54	36 853.56	52.39	36 536.07	34.98	36 307.14*	06.07	35 993.96*	993.08
55	31.00	29.92	08.01	07.05	284.08	282.92	65.78*	64.64*
56	07.88	06.68	479.48	478.39	60.47	59.33	36.81	35.63
57	784.14	782.90	50.50	49.37	36.44	35.27	07.34	06.21
58	59.88	58.76	21.05	19.84	11.51	10.32	877.31	876.13
59	35.15	33.97	390.97	389.78	185.99	184.97	46.85	45.65
60	09.89	08.69	60.41	59.23	60.26	59.08	15.80	14.56
61	684.08	682.85	29.30*	28.10	33.98	32.78	784.27	783.03
62	57.71	56.52	297.70*	296.38*	07.15	05.90	52.22	50.98
63	30.89	29.68	65.52	64.27	079.65	078.46		
64	03.44	02.18	32.86	31.64	51.67	50.45		
65	575.45	574.05	199.72	198.45	23.40*	21.75*		
66	46.81	45.48	65.94	64.60	35 994.27*	993.04*		
67	17.73	16.28	31.76	30.35	64.68*	64.26		
68	488.00	486.63	096.93	095.60	34.03*	32.74*		
69	57.69	56.32	61.63	60.24	03.05	—		
70	26.79	25.39	25.69	24.31	871.58	870.41		
71	395.31	394.00	35 989.24	987.99	41.36*	39.82		
72	63.36	61.94	52.19	50.83	08.71	06.94		
73	30.77	29.40*	14.75	13.36	776.65*	775.39		
74	297.70*	296.32			43.94*	42.71		
75	63.89*	62.31*						
76	29.45*	27.87*						
77	194.52	193.01						
78	59.15	57.59						

$G(v_2) - G(v_1)$ for all combinations was obtained when the left-hand-side of these equations added with $\alpha\, K(K+1)$ were plotted against $K(K+1)$. The linear deviation gives a correction to α, a square deviation (only observable at high $K(K+1)$ values) gives β.

The rotational constants thus derived are collected in Table 6. The B'' values differ slightly from those derived by Jenkins and McKellar (1932). They obtained $B_v'' = 1.7803 - 0.01648\ (v + \frac{1}{2})$.

The difference between the spin doubling constants $\gamma' - \gamma''$ has been determined from the expressions

$$\Delta\nu P_{12}(K),\ \Delta\nu R_{12}(K) \text{ and } \tfrac{1}{2}\,[\Delta\nu R_{12}(K-1) + \Delta\nu P_{12}(K)].$$

The results are

$$\gamma_0' - \gamma_0'' = 0.02_1\ \text{cm}^{-1} \qquad \gamma_1' - \gamma_0'' = 0.02$$

$$\gamma_0' - \gamma_1'' = 0.01_9 \qquad \gamma_1' - \gamma_4'' = 0.02_0$$

$$\gamma_0' - \gamma_2'' = 0.01_9 \qquad \gamma_2' - \gamma_2'' = 0.02$$

$$\gamma_0' - \gamma_3'' = 0.02_0$$

Table 4. Wavenumbers for the lines of the 2,0 and 2,2 bands.

K	2,0				2,2			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
9	45 372.5*		45 317.2*				41 618.4*	
10	69.8*		08.5*				10.6*	
11	65.8*		297.8*				02.4*	
12	61.2*		88.2*				593.4	593.3
13	56.5*		77.2*		41 662.2*	661.3*	83.5	83.2
14	50.4*		65.3*		57.8	57.3	72.7	72.2
15	43.9*		53.3*		52.0	51.4	61.4*	
16	37.6	36.7	40.5*		46.1	45.7	49.7	49.3
17	29.4*		26.9*		39.5	39.1	37.3*	
18	21.8	20.9	13.8*		32.6	32.1	24.6	24.2
19	12.5	11.7	—		24.8	24.3	11.4*	11.0*
20	02.8*	01.7*	182.8*		17.0	16.5	497.2	496.6
21	292.6	291.7	67.0*		07.9	07.4	82.7	82.3*
22	82.5*	81.1*	50.3*		598.5	597.9	67.4	67.0
23	71.1*	70.0*	33.9	32.9	88.6	88.0	51.7	51.0
24	59.1*	57.8*	15.5		78.1	77.4*	35.5	35.0
25	45.5*		097.1	—	67.1	66.2	18.7	18.1
26	31.8*		—	077.6	55.5	54.8	01.4	00.6
27	—	—	—	58.0	43.2	42.4	383.5	382.9
28	03.4*		38.1	37.3	30.5	29.9	65.1	64.3
29	188.1*		17.5	16.6	17.1	16.3	45.9	45.3
30	172.3	171.4	44 995.3	—	03.1	02.3	26.3	25.7
31	56.3	55.2	73.7	44972.4	488.6	487.8	06.1	05.5
32	38.8	37.5	50.8	49.9	73.4	72.7	285.4	284.6
33	21.1	20.0	27.0*	—	57.8*	57.0	64.0	63.3
34	02.1	00.8	02.5	—	41.5	40.8	42.1	41.3
35	083.1	082.6	878.1	877.2	24.5	24,0	19.6	19.1*
36	63.2	62.0	52.9	51.8	07.1	06.5*	196.6	195.9
37	42.7	41.6	27.1*	26.1	388.6	387.9*	72.9*	72.4
38	21.7	20.3*	799.9*	799.0	70.4	69.6	48.7	48.1
39	44 999.6	998.8	73.1*	72.0*	51.3	50.5	24.1	23.4
40	77.5	76.2	44.6*	43.5*	31.5	30.7*	098.9*	098.0
41	54.2	53.0	15.7*	14.5*	10.9	10.1*	72.8*	72.0
42	30.2	29.2	686.4*	685.3*	289.8	289.0	46.3*	45.3*
43	06.1	04.6	56.8*	55.6*	68.4	67.4		
44	880.9	879.7	26.3	25.3	46.2	45.3*		
45	54.7	53.8	594.7	593.3	23.2	22.2		
46	28.5	27.1*	63.0	61.9	199.9	198.9		
47	01.2	799.9*	30.2	29.0	75.8	74.8		
48	773.4*	72.2*	497.3	496.1	51.2	50.1		
49	44.7*	43.5*	62.9	62.3	25.9*	25.0*		
50	15.7*	14.5*	28.6	27.6	099.9	098.9*		
51	686.0*	684.6	393.5	392.4	73.6	72.7*		
52	55.2*	54.1	57.5	56.3	46.3*	45.3*		
53	24.0	22.8	20.7	19.8				
54	592.0	590.8	283.6	282.7				
55	59.2	57.9	45.6	44.5				
56	26.0	24.5	07.1	05.8				
57	491.9	490.5*	167.8*	166.3*				
58	—	56.8	27.6	26.5				
59	21.2	20.4*	087.1	085.7				
60	385.3	384.1	45.6	43.9*				
61	48.4*	47.1	03.6	02.2				
62	11.1	09.6	43 960.9	959.4				
63	272.6	271.0						

Table 5. Wavenumbers for the lines of the 3,1 band.

K	3.1			
	$R_1(K)$	$R_2(K)$	$P_1(K)$	$P_2(K)$
25	44 597.1*		44 451.2*	
26	83.5*		31.4*	
27	69.4*		—	
28	55.1*		390.5*	
29	39.5	38.8	—	
30	—	23.1	—	
31	06.8*		326.5*	325.6*
32	—	489.0	04.2*	03.0*
33	71.3*		280.3*	
34	53.3	52.3	56.1*	
35	33.8	33.0	32.1	30.6
36	13.7	12.8	05.8*	
37	—	—	179.4*	
38	371.4*		52.6*	
39	49.9*			
40	27.7	26.5*		
41	04.2*	03.0*		
42	280.3	278.9		
43	54.3	53.2		
44	27.9	26.3		

As no difference in the F_1 and F_2 combination differences has been observed in the upper as well as in the lower state it is impossible to settle the absolute values of γ' and γ''. They must, however, be small.

The origins derived by (1) are given in Table 7. The vibrational constants—determined by use of (2) and (3)—are also given there. In order to get as good constants as possible all combinations of the bands have been used in this calculation.

Table 6. Rotational constants of the $B\,^2\Sigma$ and $X\,^2\Sigma$ states of BO in cm^{-1}.

v	B_v'	B_v''	$D_v' \times 10^6$	$D_v'' \times 10^6$
0	1.5066	1.7737	8.51	6.34
1	1.4856	1.7570	8.46	6.35
2	1.4646	1.7405	8.3	6.37
3	1.445	1.7239		6.39
4		1.7076		6.41

$B_v' = 1.5171 - 0.0210\,(v + {}^1/_2)$
$D_e' \approx 8.5 \times 10^{-6}$
$r_e' = 1.3053 \times 10^{-8}$ cm

$B_v'' = 1.7820 - 0.0166\,(v + {}^1/_2)$
$D_v'' = [6.32 + 0.02\,(v + {}^1/_2)] \times 10^{-6}$
$r_e'' = 1.2043 \times 10^{-8}$ cm

Table 7. Origins of analysed β-bands in cm^{-1}.

v' ↑ / v'' →	0		1		2		3	4
2	45 371.45				41 671.53			
	1238.83							
1	44 132.62							36 826.32
	1260.36							
0	42 872.26	1862.01	41 010.35	1838.45	39 171.80	1814.85	37 356.95	

$$\omega_e'' = 1885.69 \qquad \omega_e' = 1281.69$$

$$\omega_e'' x_e'' = 11.81 \qquad \omega_e' x_e' = 10.66$$

$$T_e = 43174.05$$

Survey of spectroscopic data on BO

The present position of spectroscopic work on BO is as follows. Only the α-system, $A\,^2\Pi - X\,^2\Sigma^+$, and now the β-system $B\,^2\Sigma^+ - X\,^2\Sigma^+$ have been investigated with aspect to the rotational structure. The combination system $B\,^2\Sigma^+ - A\,^2\Pi$ was found by Mulliken (1925), who measured some heads. Further Chrétien (1950) has observed a system situated in the ultraviolet which probably arises from a $^2\Pi - X\,^2\Sigma$ transition. The head formula is

$$\nu_{v'v''} = 56670 + 1300\,(v' + \tfrac{1}{2}) - 15\,(v' + \tfrac{1}{2})^2 - 1886\,(v'' + \tfrac{1}{2}) + 14\,(v'' + \tfrac{1}{2})^2.$$

Singh (1949) has reported another system in the visible region, which he considers to be a transition between an excited $^2\Sigma$ state and the $B\,^2\Sigma$ state. He has given the following head equation

$$\nu_{v'v''} = 21030 + 1193.3\,v' - 14.3\,v'^2 - 1268.8\,v'' + 9.98\,v''^2.$$

The constants for BO are collected in Table 8.

Table 8. Data of electronic states in BO.

Electronic state	T_e	ω_e	$\omega_e x_e$	B_e	α_e	$D_e \times 10^6$	r_e	Transition
$D\,^2\Sigma$ (?)	64 240	1208	14.3					$D \to B$
$C\,^2\Pi$ (?)	56 670	1300	15					$C \to X$
$B\,^2\Sigma$	43 174.0	1281.69	10.66	1.5171	0.0210	8.5	1.3053	$D \to B$ $B \to A$ $B \to X$
$A\,^2\Pi$	23 958.85 23 836.49	1260.70	11.157	1.4132	0.0196	7.09	1.3524	$B \to A$ $A \to X$
$X\,^2\Sigma$	0	1885.69	11.810	1.7820	0.0166	6.32	1.2043	$C \to X$ $B \to X$ $A \to X$

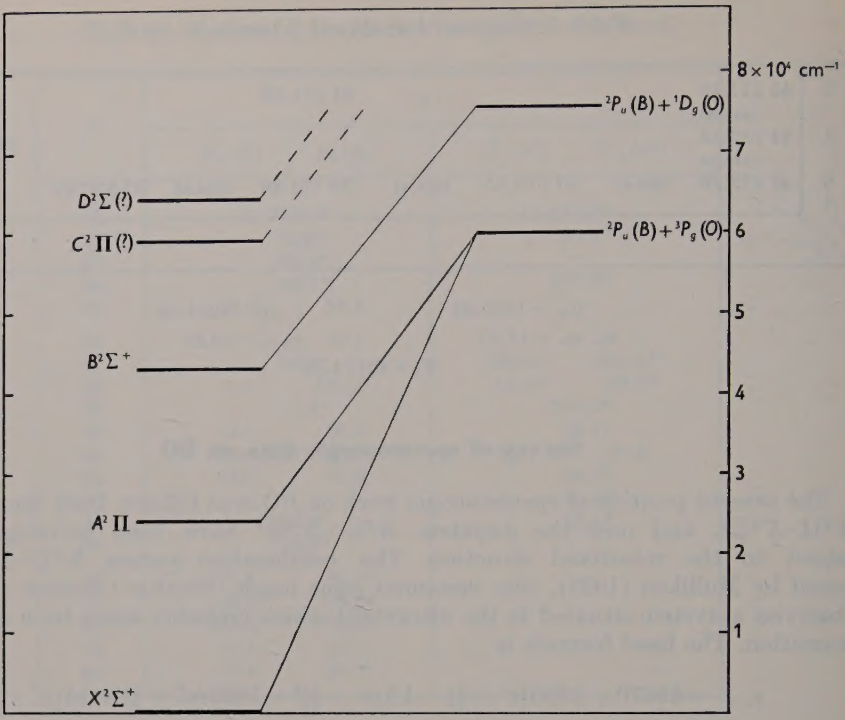

Fig. 2. Energy level scheme of BO.

The dissociation energy of BO is estimated by Gaydon (1957) to 7.6 ± 0.4 e.v. Using the approximate formula

$$D_e = \frac{\omega_e^2}{4\, x_e\, \omega_e}$$

for the three states $X\,^2\Sigma^+$, $A^2\Pi$ and $B\,^2\Sigma^+$, we obtain, if we assume that X and A go to the atomic ground states $^2P_u(\mathrm{B}) + {}^3P_g(\mathrm{O})$ and B goes to $^2P_u(\mathrm{B}) + {}^1D_g(\mathrm{O})$, following values for D_e; 75000 cm⁻¹, 60000 cm⁻¹ and 66000 cm⁻¹. The lowest value 60000 cm⁻¹ corresponds to 7.4. e.V.

Fig. 2 gives the energy level scheme of BO.

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